

Link between New Versions of the Hierarchical Reference Theory of Liquids and of the Non Perturbative Renormalization Group in Statistical Field Theory

Jean-Michel Caillol
 LPT (UMR 8627)
 Bât. 210
 Université de Paris-Sud
 F-91405 Orsay CedexFrance
 and
 CNRS, Orsay, F-91405, France

June 28, 2011

Abstract

I propose a new version of the Hierarchical Reference Theory of liquids. Two formalisms, one in the grand canonical ensemble, the other in the framework of statistical field theory are given in parallel. In the latter the theory is an avatar of a new version of the non perturbative renormalization group (J. Phys. A : Math. Gen. **42**, 225004 (2009)). The flow of the Wilsonian action as well as that of the effective average action of Wetterich are derived and a simple relation between the two functionals is established. The standard Hierarchical Reference Theory for liquids (*Adv. Phys.* **44**, 211 (1995)) is recovered for a sharp infra-red cut-off of the propagator

key-words :statistical field theory; non-perturbative renormalization group; theory of liquids; hierarchical reference theory.

Contents

1	Introduction	3
2	The model	4
2.1	Grand-Canonical representation	4
2.2	Field theoretical representation	5
3	Coarse graining	7
3.1	Ultra-violet regularization of the pair potential	7
3.2	Two lemma	8
3.3	Blocking the action	9
4	RG Flow equations	11
4.1	RG flow of the grand potential W_k^Λ	11
4.2	RG flow of the Wilsonian action S_k^Λ	12
4.3	RG flow of the effective average Kohn-Sham free energy $\beta\mathcal{A}_k^\Lambda$.	13
5	Conclusion	16
A	Alternative derivation of the RG flow of W_k^Λ	18
B	Mean field theory at scale “k”	18

1 Introduction

The first theory of liquids which incorporates the ideas of the renormalization group (RG) of Wilson [1, 2] was proposed more than twenty-five years ago in a series of outstanding papers by Reatto, Parola and co-workers who developed the so-called Hierarchical Reference Theory (HRT) which gives an accurate description of the thermodynamics and the structure of a wide class of fluids close to and away from the critical region [3, 4, 5, 6, 7]. The theory was developed and improved over years by these authors until very recently.

During roughly the same period the Wilson approach to the (RG) has been the subject of a revival in both statistical physics and field theory. Two main formulations of the non perturbative renormalization group (NPRG) have been developed in parallel. In the first one, the RG transformations concern the Hamiltonian (or action) of the model [1, 2, 8, 9, 10] while, in the second, the RG flow of the free energy is under scrutiny, or rather, to be more precise, the so-called "effective average action" [11, 12]. In both approaches, at scale " k " (in momentum space), a cut-off is introduced to separate the slow ($q < k$) and the fast ($q > k$) modes of the field. In the first approach the Wilsonian action is defined to be the effective action of the low energy modes yielding the same physics a long distances than the bare action. In this case the cut-off acts as an ultra-violet (UV) cut-off. In the formalism of Wetterich these ideas are implemented at the level of the Helmholtz free energy of the fast modes (in fact one is rather interested in its Legendre transform, the effective average action) and thus, in this approach, the cut-off acts conversely as an infra-rouge (IR) cut-off. The two points of view can be reconciliated formally [10, 13].

It turns out that many of new results obtained recently for the NPRG had been anticipated by the seminal works of Reatto 'et al.'. Since the two communities have few contacts and use a different language many things have been discovered or rediscovered independently by both sides in the ignorance of the results obtained by the other camp. Today field theorists would say that HRT is a sharp cut-off version of Wetterich effective average action approach to the RG, while specialists of liquids would claim that Wetterich theory is nothing but a field theoretical version of HRT with smooth cut-off and strange notations.

A precise comparison between the two worlds however requires a field theoretical representation of simple classical liquids. Technically, a simple Hubbard-Stratonovich transform does the job [14, 15]. This has been realized by many authors [16, 17, 18, 19]. The more achieved scalar field theoretical representation of liquids at equilibrium has been christened the KSSHE theory after the names of Kac [20], Siegert [21], Stratonovich [14], Hubbard [15]

and Edwards [22] and is developed in references [18, 19] *inter alia*. I show in the latter reference that the implementation of Wetterich effective average action method in the framework of KSSHE theory yields indeed HRT in the ultra-sharp cut-off limit.

In general the field theory obtained via a Hubbard-Stratonovich transform yields a non-canonical theory in the sense that the coupling between the field φ and the source, here the chemical potential ν , is non linear (see section 2.2 below). An additional transformation is needed to obtain a standard field theory with a linear coupling. I adhered to this method in my previous works on liquids [18, 19]. However it turns out that the NPRG ideas can easily be extended to the non-canonical theory itself and it has then the advantage to yield extremely simple functional relationships between the Wilsonian action and Wetterich's effective average action [13]. In the present paper I will show that applying this new field theoretical formalism to the KSSHE theory leads to a slightly different version of HRT with some advantages however. For instance the flow equations of Reatto 'et al' are reobtained by taking the limit of an ordinary sharp cut-off. Moreover the grand-canonical functionals corresponding to the Wilsonian and effective average actions of Wetterich are clearly identified which allows a deeper understanding of the NPRG for liquids.

The paper is organized as follows. In next section 2, I circumscribe the type of liquids under study (the simplest!) and give their representations in the grand-canonical ensemble and in field theory. Then, in section 3, the coarse-graining operations of the various functionals of interest are detailed and their flow equations are derived in section 4. in the last paragraph 4.3, the usual HRT equation is obtained by taking the limit of a sharp cut-off. We summarize and conclude in section 5. Two appendices explain some technical points.

2 The model

2.1 Grand-Canonical representation

I consider a classical simple fluid made of identical hard spheres (HS) of diameter σ with, in addition, isotropic pair interactions $v(r_{ij})$ ($r_{ij} = |x_i - x_j|$, x_i position of particle "i"). Since $v(r)$ can be chosen arbitrarily in the core, we assume that $v(r)$ has been regularized for $0 < r < \sigma$ in such a way that its Fourier transform \tilde{v}_q is a well behaved function of q and that $v(0)$ is a finite quantity. For convenience the domain $\Omega \subset \mathbb{R}^d$ occupied by the molecules is chosen to be a d -dimensional cube of side L within periodic boundary (PB)

conditions; the volume of Ω is noted $V = L^d$. The fluid is at equilibrium in the grand canonical (GC) ensemble, $\beta = 1/k_B T$ is the inverse temperature (k_B Boltzmann's constant), and μ the chemical potential. In addition the particles are subject to an external potential $\psi(x)$ and we will denote by $\nu(x) = \beta(\mu - \psi(x))$ the dimensionless local chemical potential. I adhere to notations usually adopted in standard textbooks on liquids (see e.g. [23]) and thus denote by $w(r) = -\beta v(r)$ *minus* the dimensionless pair interaction. Moreover we restrict ourselves to the case of **attractive** interactions, i.e. such that $\tilde{w}(q) > 0$ for all q . The model admits a thermodynamic limit if $w(r)$ decays faster than $1/r^{d+\epsilon}$ as $r \rightarrow \infty$, where d is the space dimensions and $\epsilon > 0$ [24].

In a given GC configuration $\mathcal{C} \equiv (N; x_1 \dots x_N)$ the microscopic density of particles at point x reads

$$\hat{\rho}(x|\mathcal{C}) = \sum_{i=1}^N \delta^{(d)}(x - x_i) , \quad (1)$$

and the grand canonical partition function (GCPF) $\Xi[\nu]$ which encodes all the physics of the model at equilibrium is defined as [23]

$$\begin{aligned} \Xi[\nu] &= \text{Tr} [\exp(-\beta \mathcal{H}[\mathcal{C}])] , \\ -\beta \mathcal{H} &= \frac{1}{2} \hat{\rho} \cdot w \cdot \hat{\rho} + \left(\nu - \frac{w(0)}{2} \right) \cdot \hat{\rho} , \\ \text{Tr} [\dots] &= \sum_{N=0}^{\infty} \frac{1}{N!} \int_{\Omega} d1 \dots dn \exp[-\beta V_{(\text{HS})}[\mathcal{C}]] \dots , \end{aligned} \quad (2)$$

where $i \equiv x_i$ and $di \equiv d^d x_i$. In equation (2) $\beta V_{(\text{HS})}[\mathcal{C}]$ denotes the HS contribution to the configurational integral. Its Boltzmann factor is either 0 if configuration \mathcal{C} involves overlaps of spheres, or 1 otherwise. Note that in fact $\Xi[\nu]$ does not depend on the self energy $-w(0)/2$. For a given volume V and a given inverse temperature β , $\Xi[\nu]$ is a log-convex functional of the local chemical potential $\nu(x)$ [25, 26]. I have employed here convenient matricial notations.

$$\bar{\nu} \cdot \hat{\rho} \equiv \int_{\Omega} d^d x \bar{\nu}(x) \hat{\rho}(x|\mathcal{C}) \quad (3)$$

$$\hat{\rho} \cdot w \cdot \hat{\rho} \equiv \int_{\Omega} d^d x d^d y \hat{\rho}(x|\mathcal{C}) w(x, y) \hat{\rho}(y|\mathcal{C}) . \quad (4)$$

2.2 Field theoretical representation

It is possible to express $\Xi[\nu]$ as a functional integral making thus a link between the theory of liquids and statistical field theory [16, 17, 18]. With

the help of a Hubbard-Stratonovich transform [14, 15] one gets:

$$\Xi[\nu] = \mathcal{N}_w^{-1} \int \mathcal{D}\varphi \exp \left(-\frac{1}{2} \varphi \cdot R \cdot \varphi + W_{(\text{HS})} [\nu - w(0)/2 + \varphi] \right) \quad (5)$$

where $W_{(\text{HS})} \equiv \ln \Xi_{(\text{HS})}$, φ is a real random scalar field, $R \equiv w^{-1}$ is the inverse of w (in the sense of operators, i.e. $w(1, 3) \cdot R(3, 2) = \delta^{(d)}(1, 2)$) and $\Xi_{(\text{HS})} [\nu - w(0)/2 + \varphi]$ denotes the GCPF of bare hard spheres in the presence of a local chemical potential $\nu(x) - w(0)/2 + \varphi(x)$. We optimistically suppose that the functional $\Xi_{(\text{HS})} [\nu]$ as well as its functional derivatives, *i. e.* the density-density correlation functions, are known exactly. This is *nearly* true since the HS fluid has been under scrutiny since so many years [23].

I have noted \mathcal{N}_w the normalization constant

$$\mathcal{N}_w = \int \mathcal{D}\varphi \exp \left(-\frac{1}{2} \varphi \cdot R \cdot \varphi \right) . \quad (6)$$

The functional integrals which enter equations (5) and (6) can be given a precise meaning in the case where the domain Ω is a cube of side L with periodic boundary conditions, in this case the measure $\mathcal{D}\varphi$ reads [2]

$$\mathcal{D}\varphi \equiv \prod_{q \in \Lambda} \frac{d\tilde{\varphi}_q}{\sqrt{2\pi V}} \quad (7a)$$

$$d\tilde{\varphi}_q d\tilde{\varphi}_{-q} = 2 d\Re \tilde{\varphi}_q d\Im \tilde{\varphi}_q \text{ for } q \neq 0 . \quad (7b)$$

where $\Lambda = (2\pi/L) \mathbb{Z}^D$ (\mathbb{Z} ring of integers) is the reciprocal cubic lattice. Note that the reality of φ implies that, for $q \neq 0$, $\tilde{\varphi}_{-q} = \tilde{\varphi}_q^*$, where the star means complex conjugation. With this slick normalization of the functional measure one has exactly

$$\mathcal{N}_w = \exp \left(\frac{V}{2} \int_q \ln \tilde{w}(q) \right) \quad (8)$$

in the limit of large systems ($L \rightarrow \infty$).

The field theoretical representation (5) of the GCPF $\Xi[\nu]$ can be extended to arbitrary pair potentials. If $w(1, 2)$ contains a definite negative part corresponding to a repulsive interaction then a second scalar field, purely imaginary must be introduced via an additional Hubbard-Stratonovich transform, see e.g. ref [18]. Handling these two fields makes the algebra a little bit more complicated but by no means intractable; we lazily skip this complication in this paper and restrict ourselves to attractive $w(r)$. Alternatively, one can gather the HS and repulsive pair potentials contributions in a single functional $W_{(\text{Ref})}$ which will play the role devoted to $W_{(\text{HS})}$.

It is important to note that (5) “looks” like the generator of Green’s function of a field theory with an action $\mathcal{S}[\varphi] = \frac{1}{2}\varphi \cdot w^{-1} \cdot \varphi - W_{(\text{HS})}[\nu - w(0)/2 + \varphi]$, with $w(1, 2)$ playing the role of the bare propagator and the non local term $W_{(\text{HS})}$ that of the interaction. However purists will note that this is not a “canonical” field theory *stricto sensu* since the coupling between the field φ and the external source ν is non-linear. As detailed at length in refs. [19, 13] this point can be circumvented by the change of variables $\chi = \varphi + \nu - w(0)/2$. By doing so one recovers a “canonical” field theory involving a linear coupling between χ and ν . Moreover one can establish a rigorous mapping between these two field theories. Then all the knowledge amassed in statistical field theory can be injected in the theory of liquids, notably well established perturbative technics and/or more recent non-perturbative approaches. Recently however we proposed rather to consider the action $\mathcal{S}[\varphi]$ as a well-educated one and work directly with it rather than to try to scholarly adhere to a canonical action via the mapping $\varphi \leftrightarrow \chi$. As discussed in reference [13], the adoption of this “non-canonical” point of view leads to a remarkably simple reconciliation between the points of view of Wilson-Polchinski on the one hand and that of Wetterich in the other hand. Applied to liquids, as will be done here, it yields a new version of the smooth HRT theory with some advantages on my previous attempts [19].

3 Coarse graining

The coarse graining procedure involved to build families of actions with the same physics at long distances is the core of the RG theory. In this section we introduce this procedure step-by-step following recent developments in field theory [10, 13]

3.1 Ultra-violet regularization of the pair potential

I noted in section 2.1 that the pair potential (propagator) $w(r)$ can be regularized at short distances $0 < r < \sigma$, *i. e.* in the ultra-violet (UV) regime, without changing the GCPF $\Xi[\nu]$ of the system. I introduce a potential $w_0^\Lambda(r)$ defined in Fourier space by

$$\tilde{w}_0^\Lambda(q) = C(q, \Lambda) \tilde{w}(q) , \quad (9)$$

where $C(q, \Lambda)$ is an UV cut-off which is equal to 1 for $q < \Lambda$ and to 0 for $q > \Lambda$. Typically $C(q, \Lambda) = 1 - \Theta_\epsilon(q, \Lambda)$ where $\Theta_\epsilon(q, \Lambda)$ is a function which looks like the step function $\Theta(q - \Lambda)$. It could be precisely this function and we would then speak of a sharp cut-off; or it could be a smooth version

with $\Theta_\epsilon(q, \Lambda)$ varying smoothly from 0 to 1 in a small interval $(\Lambda - \epsilon, \Lambda + \epsilon)$ about the UV cut-off; in this case we would speak of a smooth UV cut-off. It is sometimes convenient to choose $C(q, \Lambda) = \overline{C}(x = q/\Lambda)$ but by no means compulsory.

In any case if $\Lambda\sigma \gg 1$ then $w(r)$ and $w_0^\Lambda(r)$ coincide outside the core and moreover we have $\tilde{w}_0^\Lambda(0) = \tilde{w}(0)$ and $|w_0^\Lambda(r=0)| < \infty$. Although this UV regularization does not change the GCPF $\Xi[\nu]$ we shall henceforth note this functional $\Xi_0^\Lambda[\nu]$ to emphasize that it depends functionally on w_0^Λ . For further convenience, we also need a special notation for the inverse of the regularized propagator w_0^Λ which will be christened $R_0^\Lambda = [w_0^\Lambda]^{-1}$. We can thus rewrite (2) and (5) as

$$\Xi_0^\Lambda[\nu] = \text{Tr} \left[\exp \left(\frac{1}{2} \hat{\rho} \cdot \tilde{w}_0^\Lambda \cdot \hat{\rho} + \hat{\rho} \cdot [\nu - w_0^\Lambda(0)/2] \right) \right], \quad (10a)$$

$$= \frac{1}{\mathcal{N}_{w_0^\Lambda}} \int \mathcal{D}\varphi \exp \left(-\frac{1}{2} \varphi \cdot R_0^\Lambda \cdot \varphi + W_{(\text{HS})} [\nu - w_0^\Lambda(0)/2 + \varphi] \right) \quad (10b)$$

Of course $\Xi_0^\Lambda[\nu] \equiv \Xi[\nu]$ as soon as $\Lambda\sigma \gg 1$ which will be assumed.

3.2 Two lemma

I prefer, for the convenience of the reader, to give here two lemma necessary for subsequent developments rather than to postpone them in an appendix. Let Δ some definite positive operator and $\mathcal{F}[\varphi]$ an arbitrary functional of real scalar field φ , then

$$\frac{1}{\mathcal{N}_\Delta} \int \mathcal{D}\varphi \exp(-\frac{1}{2} \varphi \cdot \Delta^{-1} \cdot \varphi) \mathcal{F}[\varphi + \varphi_0] = \exp(D_0) \mathcal{F}(\varphi_0), \quad (11)$$

where the operator D_0 reads

$$D_0 \dots = \frac{1}{2} \int_\Omega d^d x d^d y \Delta(x, y) \frac{\delta^2 \dots}{\delta \varphi_0(x) \delta \varphi_0(y)}. \quad (12)$$

An interesting application of lemma (11) is to reconsider equation (10b) as

$$\Xi_0^\Lambda[\nu + w_0^\Lambda(0)/2] = e^{D_0^\Lambda} \Xi_{(\text{HS})}[\nu], \quad (13)$$

therefore the operator $e^{D_0^\Lambda}$ constructs the full GCPF of the system from the GCPF of the reference HS system.

The second lemma is sometimes referred to as Bogolioubov theorem :

Let Δ_i , $1 \leq i \leq n$, be n definite positive operators and $\mathcal{F}[\varphi]$ an arbitrary functional of real scalar field φ , then

$$\int \prod_{i=1}^n \left\{ \frac{\mathcal{D}\varphi_i}{\mathcal{N}_{\Delta_i}} \exp\left(-\frac{1}{2}\varphi_i \cdot \Delta_i^{-1} \cdot \varphi_i\right) \right\} \mathcal{F}\left(\sum_{i=1}^n \varphi_i\right) = \int \frac{\mathcal{D}\varphi}{\mathcal{N}_{\Delta}} \exp\left(-\frac{1}{2}\varphi \cdot \Delta^{-1} \cdot \varphi\right) \times \mathcal{F}(\varphi), \quad (14)$$

where $\Delta = \sum_{i=1}^n \Delta_i$.

The two lemma (11) and (14) are easy consequences of Wick's theorem.

3.3 Blocking the action

I now apply the exact RG approach of Tim Morris [10, 13] to our non-canonical field theory. As a consequence of Bogolioubov theorem (14) the GCPF $\Xi_0^\Lambda[\nu]$ can be rewritten in terms of two propagators and two fields as

$$\Xi_0^\Lambda[\nu] = \frac{1}{\mathcal{N}_{w_0^k}} \int \mathcal{D}\varphi_{<} \exp\left(-\frac{1}{2}\varphi_{<} \cdot R_0^k \cdot \varphi_{<}\right) \Xi_k^\Lambda[\nu - w_0^k(0)/2, \varphi_{<}] , \quad (15a)$$

$$\begin{aligned} \Xi_k^\Lambda[\nu, \varphi_{<}] &= \frac{1}{\mathcal{N}_{w_k^\Lambda}} \int \mathcal{D}\varphi_{>} \exp\left(-\frac{1}{2}\varphi_{>} \cdot R_k^\Lambda \cdot \varphi_{>} + \right. \\ &\quad \left. + W_{(\text{HS})}\left[\nu - \frac{w_k^\Lambda(0)}{2} + \varphi_{<} + \varphi_{>}\right]\right) , \end{aligned} \quad (15b)$$

where $0 \leq k \leq \Lambda$ is the running scale of the RG and where

$$\varphi = \varphi_{<} + \varphi_{>} \text{ and } w_0^\Lambda = w_k^\Lambda + w_0^k. \quad (16)$$

In (15)-(16) I have separated the field φ into “rapid” ($\varphi_{>}$) and “slow” modes ($\varphi_{<}$). The low-energy modes are associated to the propagator w_0^k (with inverse R_0^k) which is cut off from above by k , while the high-energy modes are associated to the propagator w_k^Λ (with inverse R_k^Λ) which is cut off from below by k and from above by Λ . I demand that $\tilde{w}_k^\Lambda(q) = \tilde{w}_0(q)(C(q, \Lambda) - C(q, k))$ should be positive which will be assumed henceforth. In the popular case where $C(q, \Lambda) = \overline{C}(q/\Lambda)$ it is sufficient for the cut-off function $\overline{C}(x)$ to be a monotonous decreasing function of its argument. Some comments are in order.

- (i) In order to establish equations (15) I used $w_0^\Lambda(0) = w_k^\Lambda(0) + w_0^k(0)$ as implied by (16).

- (ii) Note that the “slow” and “rapid” modes, respec. $\varphi_<$ and $\varphi_>$ are ordinary scalar fields, in particular they have a full spectrum of Fourier components $\tilde{\varphi}_<(q)$ and $\tilde{\varphi}_>(q)$ (even the condition $0 \leq q \leq \Lambda$ is not compulsory if the bare propagator is UV regularized). The cut-off at scale “k” acts only on the propagators.
- (iii) The functional $\Xi_k^\Lambda[\nu, \varphi]$ noted in this way by Morris [10] is the crux of the whole matter since it allows, as I will show, to make explicit the link between the Wilsonian action and the effective average action. However here this link proves trivial since, as apparent in formula (15b), $\Xi_k^\Lambda[\nu, \varphi]$, depends functionally only on the sole variable $\nu + \varphi$.

Let me first set $\varphi_< = 0$ in (15b). It yields

$$\Xi_k^\Lambda[\nu, \varphi_< = 0] \triangleq \Xi_k^\Lambda[\nu] (\triangleq \exp(W_k^\Lambda[\nu])) \quad (17a)$$

$$= \frac{1}{\mathcal{N}_{w_k^\Lambda}} \int \mathcal{D}\varphi \exp\left(-\frac{1}{2}\varphi \cdot R_k^\Lambda \cdot \varphi + W_{(\text{HS})}[\nu - w_k^\Lambda(0)/2 + \varphi]\right). \quad (17b)$$

From the point of view of field theory this shows that $W_k^\Lambda[\nu] = \ln \Xi_k^\Lambda[\nu]$ is the Helmholtz free energy of the rapid modes $\varphi_>$ in the presence of the source $\nu(x)$; W_k^Λ is thus the generating functional of connected correlation functions with UV regularization (at Λ) and an infra-red (IR) cut-off (*i. e.* at k). This functional is related by a Legendre transformation to the effective average action of Wetterich, as it will be discussed in section 4.

From the point of view of the theory of liquids clearly, (see *e. g.* equation (5)) $\Xi_k^\Lambda[\nu]$ is precisely the GCPF of a system of hard spheres with additional pairwise potentials $w_k^\Lambda[r]$, *i. e.*, the k -system, to adopt the terminology of Reatto ‘et al.’ [6]. Therefore one also has :

$$\Xi_k^\Lambda[\nu] = \text{Tr} \left[\exp \left(\frac{1}{2} \hat{\rho} \cdot \tilde{w}_k^\Lambda \cdot \hat{\rho} + \hat{\rho} \cdot [\nu - w_k^\Lambda(0)/2] \right) \right]. \quad (18)$$

Note that equation (18) is valid provided the propagator $\tilde{w}_k^\Lambda(x, y)$ (pair potential) is definite positive (attractive) so that a Hubbard-Stratonovich transform is licit; that is why I imposed earlier that the cut-off function $x \rightarrow \overline{C}(x)$ should be a decreasing function. Comparing equations (15b) and (17b) one thus has synthetically

$$\Xi_k^\Lambda[\nu, \varphi] = \Xi_k^\Lambda[\nu + \varphi]. \quad (19)$$

I now introduce the Wilsonian action

$$\mathcal{S}_k^\Lambda[\varphi] \triangleq -W_k^\Lambda[\varphi], \quad (20)$$

which allows me to rewrite (15a) as

$$\Xi_0^\Lambda [\nu + w_0^k(0)/2] = \frac{1}{\mathcal{N}_{w_0^k}} \int \mathcal{D}\varphi_< \exp \left(-\frac{1}{2} \varphi_< \cdot R_0^k \cdot \varphi_< - \mathcal{S}_k^\Lambda [\nu + \varphi_<] \right) \quad (21)$$

Indeed, in equation (21) $\mathcal{S}_k^\Lambda [\varphi_<]$ play the role of the effective action of the slow modes at scale k [1, 2, 10]. Here k plays the role of an UV cut-off. Note that the functional identity $\mathcal{S}_k^\Lambda = -W_k^\Lambda$ is not true for a canonical field theory [10].

We end this section by applying lemma (11) to the 2 equations (15) which can thus be rewritten as

$$\Xi_0^\Lambda [\nu + w_0^k(0)/2] = e^{D_0^k} \Xi_k^\Lambda [\nu] \quad (22a)$$

$$\Xi_k^\Lambda [\nu + w_k^\Lambda(0)/2] = e^{D_k^\Lambda} \Xi_{(\text{HS})}^\Lambda [\nu] \quad (22b)$$

from which it follows that

$$\Xi_0^\Lambda [\nu + w_0^k(0)/2] = e^{D_0^k} e^{D_k^\Lambda} \Xi_{(\text{HS})}^\Lambda [\nu] . \quad (23)$$

Comparing with equation (13) yields

$$e^{D_0^\Lambda} = e^{D_0^k} e^{D_k^\Lambda} . \quad (24)$$

This is the semi-group law of the RG.

4 RG Flow equations

4.1 RG flow of the grand potential W_k^Λ

From the definitions (16) when $k \rightarrow \Lambda$ then $w_k^\Lambda(r) \rightarrow 0$ and the k -system at $k = \Lambda$ is a fluid of hard spheres. When k decreases from Λ to $k = 0$ more and more Fourier components are included in the potential $w_k^\Lambda(r)$ and finally precisely at $k = 0$ the k -system coincides with the full model since $w_k^\Lambda(r)$ tends to $w_0^\Lambda(r)$, *i. e.* essentially $w(r)$ since both potentials differ only in the hard cores with no effect on the physics. In this section I establish the equations which govern the flow of the grand potential W_k^Λ introduced in Sec 3 and its Legendre transform. The flow equations of the Wilsonian action \mathcal{S}_k^Λ follows trivially. Note that the formal solution of the not yet established flow equation for W_k^Λ is already known, it is given by equation (22b).

The flow equation for W_k^Λ can be obtained in the framework of statistical field theory and, apart some tricks due to the self-energies, along essentially

the same lines as in reference [13]. I postpone this derivation to appendix 5 and I give here only the proof in the framework of liquid theory. An easy task. The starting point is equation (18) which I differentiate with respect to k at fixed $\nu(x)$. It gives readily

$$\partial_k W_k^\Lambda[\nu] \big|_\nu = \frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_k^\Lambda(x, y) \{G_k^\Lambda(x, y) - \rho_k^\Lambda(x) \delta^{(d)}(x - y)\} \quad (25)$$

where $\rho_k^\Lambda(x) = \langle \hat{\rho}(x|\mathcal{C}) \rangle_{\text{GC}}$ denotes the mean density of the k -system in the GC ensemble and $G_k^\Lambda(x, y) = \langle \hat{\rho}(x|\mathcal{C}) \hat{\rho}(y|\mathcal{C}) \rangle_{\text{GC}}$ its pair correlation function at chemical potential $\nu(x)$. Since one has $\rho_k^\Lambda(x) = \delta W_k^\Lambda / \delta \nu(x) \triangleq W_k^{(1)\Lambda}(x)$ and also $G_k^{(T)\Lambda}(x, y) = G_k^{(T)\Lambda}(x, y) - \rho_k^\Lambda(x) \rho_k^\Lambda(y) = \delta^{(2)} W_k^\Lambda / \delta \nu(x) \delta \nu(y) \triangleq W_k^{(2)\Lambda}(x, y)$ one can rewrite equation (25) under the closed form

$$\begin{aligned} \partial_k W_k^\Lambda[\nu + w_k^\Lambda(0)/2] \big|_\nu &= \frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_k^\Lambda(x, y) \{W_k^{(2)\Lambda}(x, y) \\ &+ W_k^{(1)\Lambda}(x) W_k^{(1)\Lambda}(y)\}. \end{aligned} \quad (26)$$

This partial differential equation (PDE) must be supplemented by the initial condition $W_k^\Lambda \equiv W_{(\text{HS})}$. This equation is closed only superficially since the pair correlation function $W_k^{(1)\Lambda}(x)$ and $W_k^{(2)\Lambda}(x, y)$ depends functionally on the chemical potential $\nu(x)$. Differentiating functionally successively both members of equation (26) with respect to the field $\nu(x)$ one obtains a hierarchy, or tower, of equations for the $W_k^{(n)\Lambda}(x_1, \dots, x_n) = \delta^n W_k^\Lambda / \delta \nu(x_1) \dots \delta \nu(x_n)$, i. e. the Green's -or connected correlation- functions.

4.2 RG flow of the Wilsonian action S_k^Λ

The flow equation (26) has the structure of Wilson-Polchinski's equation for the Wilsonian action; indeed with $S_k^\Lambda = -W_k^\Lambda$ it takes the usual form [8, 9, 10]

$$\begin{aligned} \partial_k S_k^\Lambda[\varphi + w_k^\Lambda(0)/2] \big|_\varphi &= \frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_k^\Lambda(x, y) \{S_k^{(2)\Lambda}(x, y) \\ &- S_k^{(1)\Lambda}(x) S_k^{(1)\Lambda}(y)\}. \end{aligned} \quad (27)$$

where $S_k^{(n)\Lambda}(x_1, \dots, x_n) = \delta^n S_k^\Lambda / \delta \varphi(x_1) \dots \delta \varphi(x_n)$. This equation, which must be supplemented with the initial condition $S_\Lambda^\Lambda = -W_{(\text{HS})}$, does not appear to have yet been considered in the theory of liquids contrary to the abundant literature devoted to it in statistical field theory (see *e. g.* [9] and references quoted herein).

4.3 RG flow of the effective average Kohn-Sham free energy $\beta\mathcal{A}_k^\Lambda$

Since the seminal works of Reatto ‘et al.’ [3, 4, 5, 6] it is usual to consider rather the flow for the Kohn-Sham free energy $\overline{\mathcal{A}}_k^\Lambda[\rho]$ of the k-system which is defined as the Legendre transform of $W_k^\Lambda[\nu]$. One has the usual couple of relations

$$W_k^\Lambda[\nu] = \sup_{\rho} \left\{ \nu \cdot \rho - \beta\overline{\mathcal{A}}_k^\Lambda[\rho] \right\} \quad \forall \nu, \quad (28a)$$

$$\beta\overline{\mathcal{A}}_k^\Lambda[\rho] = \sup_{\nu} \left\{ \rho \cdot \nu - W_k^\Lambda[\nu] \right\} \quad \forall \rho. \quad (28b)$$

Obviously the flow equation for $\beta\overline{\mathcal{A}}_k^\Lambda[\rho]$ should be deduced from that of $W_k^\Lambda[\nu]$. Let me consider for instance equation (28a). I have for all ν

$$W_k^\Lambda[\nu] = \rho^* \cdot \nu - \beta\overline{\mathcal{A}}_k^\Lambda[\rho^*], \quad (29)$$

where $\rho^*(x)$ is, if it does exists, the unique solution of the implicit stationary equation

$$\nu = \frac{\delta\beta\overline{\mathcal{A}}_k^\Lambda[\rho]}{\delta\rho(x)} \Big|_{\rho=\rho^*} \quad (30)$$

Differentiating (29) at fixed ν gives

$$\partial_k W_k^\Lambda[\nu] \Big|_{\nu} = \partial_k \rho^* \cdot \nu - \frac{\delta\beta\overline{\mathcal{A}}_k^\Lambda[\rho^*]}{\delta\rho^*} \Big|_k \cdot \partial_k \rho^* - \partial_k \beta\overline{\mathcal{A}}_k^\Lambda[\rho^*] \Big|_{\rho^*}, \quad (31)$$

which further simplifies thanks to the stationary condition (30) with the final result :

$$\partial_k \overline{\mathcal{A}}_k^\Lambda[\rho^*] \Big|_{\rho^*} = - \partial_k W_k^\Lambda[\nu] \Big|_{\nu}. \quad (32)$$

Similarly, starting instead from equation (28b) one finds that

$$\partial_k \overline{\mathcal{A}}_k^\Lambda[\rho] \Big|_{\rho} = - \partial_k W_k^\Lambda[\nu^*] \Big|_{\nu^*}, \quad (33)$$

where ν^* is the unique chemical potential which is, if it exists, solution of equation (28b). I shall drop the subscript “ \star ” in the sequel.

At this point I introduce the direct correlation functions

$$\overline{\mathcal{C}}_k^{(n)\Lambda}(x_1, \dots, x_n) = -\delta^n \overline{\mathcal{A}}_k^\Lambda / \delta\rho(x_1) \dots \delta\rho(x_n), \quad (34)$$

which are the analogous to the vertex functions in field theory. I have simplified the notations and it must be stressed that, in addition to their arguments these function depend functionally on the profile $\rho(x)$. The $\bar{\mathcal{C}}_k^{(n)\Lambda}(x_1, \dots, x_n)$ and the $W_k^{(n)\Lambda}(x_1, \dots, x_n)$ are linked by generalized Ornstein-Zernike (OZ) equations and in particular one has the usual OZ equation : $W_k^{(2)\Lambda}(x, y) = -[\bar{\mathcal{C}}_k^{(2)\Lambda}]^{-1}(x, y)$ [6]. This last property allows to rewrite equation (32) in a closed form involving $\bar{\mathcal{A}}_k^\Lambda$, its functional derivatives and the propagator. One finds :

$$\begin{aligned} \partial_k \bar{\mathcal{A}}_k^\Lambda[\rho] \Big|_\rho = & -\frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_0^k(x, y) [\bar{\mathcal{C}}_k^{(2)\Lambda}]^{-1}(x, y) \\ & + \frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_0^k(x, y) \rho(x) \rho(y) - \frac{1}{2} \int_\Omega d^d x \partial_k w_0^k(x, x) \rho(x) . \end{aligned} \quad (35)$$

Note that, in order to obtain the result I made use of the trick $\partial_k w_0^k(x, y) = -\partial_k w_k^\Lambda(x, y)$. However, the resulting equation (35) is quite awkward and it is convenient, by adapting the ideas of Reatto ‘et al.’ [3, 4, 5, 6] to our case, to introduce a modified Kohn-Sham free energy :

$$\beta \mathcal{A}_k^\Lambda[\rho] = \beta \bar{\mathcal{A}}_k^\Lambda[\rho] - \frac{1}{2} \rho \cdot w_0^k \cdot \rho + \frac{1}{2} \rho \cdot w_0^k(0) . \quad (36)$$

This new functional was introduced by Wetterich ‘et al.’ [11] in statistical field theory under the name of “the effective average action” independently from Reatto ‘et al.’; it differs from $\beta \bar{\mathcal{A}}_k^\Lambda[\rho]$ by a simple quadratic form and satisfies obviously the following flow equation

$$\partial_k \mathcal{A}_k^\Lambda[\rho] = -\frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_0^k(x, y) \left\{ \mathcal{C}_k^{(2)\Lambda} - w_0^k \right\}^{-1}(x, y) \quad (37a)$$

$$\mathcal{C}_k^{(n)\Lambda}(x_1, \dots, x_n) = -\frac{\delta^n \mathcal{A}_k^\Lambda[\rho]}{\delta \rho(x_1) \dots \delta \rho(x_n)} \quad (37b)$$

I already obtained this equation in my first version of the RG group for liquids but with the help of a canonical field theory [19]. Note that the direct correlation functions $\mathcal{C}_k^{(n)\Lambda}(x_1, \dots, x_n)$ differ from the $\bar{\mathcal{C}}_k^{(n)\Lambda}(x_1, \dots, x_n)$ only for $n \geq 3$; in particular one has

$$\mathcal{C}_k^{(2)\Lambda}(x, y) = \bar{\mathcal{C}}_k^{(2)\Lambda}(x, y) + w_0^k(x, y) . \quad (38)$$

I stress that although $\beta \bar{\mathcal{A}}_k^\Lambda[\rho]$ is a convex functional of the profile $\rho(x)$ this is not the case in general for $\beta \mathcal{A}_k^\Lambda[\rho]$ except of course at $k = 0$ since $\beta \mathcal{A}_{k=0}^\Lambda[\rho] =$

$\beta \overline{\mathcal{A}}_{k=0}^\Lambda[\rho]$ as apparent in formula (36). Indeed although $\overline{\mathcal{C}}_k^{(2)\Lambda} < 0$ in the sense of operators, equation (38) shows that $\mathcal{C}_k^{(2)\Lambda}$ could become positive due to the addition of the positive operator w_0^k .

Equation (37a) must be supplemented with an initial condition at $k = \Lambda$. From $W_\Lambda^\Lambda = W_{\text{(HS)}}$ as follows from equation (22b) and $D_\Lambda^\Lambda = 0$ one concludes that $\beta \overline{\mathcal{A}}_\Lambda^\Lambda = \beta \mathcal{A}_{\text{(HS)}}$ and thus from (36)

$$\beta \mathcal{A}_\Lambda^\Lambda[\rho] = \beta \mathcal{A}_{\text{(HS)}}[\rho] - \frac{1}{2} \rho \cdot w_0^\Lambda \cdot \rho + \frac{1}{2} \rho \cdot w_0^\Lambda(0). \quad (39)$$

In KSSHE theory the initial conditions are identical but are obtained in a more complicated way which requires the divergence of the regulator at $k = \Lambda$ [19].

It turns out that the initial Kohn-Sham free energy of the k-system, *i. e.* at $k = \Lambda$, coincides with the mean-field Kohn-Sham free energy at *any* scale “k”, *i. e.* one has $\beta \overline{\mathcal{A}}_k^{\Lambda(\text{MF})}[\rho] = \beta \mathcal{A}_k^\Lambda[\rho]$ for all k. Moreover this MF free energy constitutes a rigorous upper bound to the exact free energy and thus $\beta \mathcal{A}_\Lambda^\Lambda[\rho] \geq \beta \mathcal{A}_k^\Lambda[\rho]$. This result already obtained in references [18, 19] for the KSSHE theory is proved for this new version of the theory in appendix A where a precise definition of the MF approximation is provided.

For a homogeneous system $\beta \mathcal{A}_k^\Lambda[\rho] = V f_k^\Lambda(\rho)$ where β times the free energy per unit volume $f_k^\Lambda(\rho)$ is a function (not a functional) of ρ and the flow equation for $f_k^\Lambda(\rho)$ is easily deduced from equation (37a) and reads

$$\partial_k f_k^\Lambda = -\frac{1}{2} \int_q \frac{\partial_k \tilde{w}_0^k(q)}{\tilde{\mathcal{C}}_k^{(2)\Lambda}(q) - \tilde{w}_0^k}, \quad (40)$$

where $\int_q \equiv \int d^d q / (2\pi)^d$ and $\tilde{\mathcal{C}}_k^{(2)\Lambda}(q)$ is the Fourier transform of $C_k^{(2)\Lambda}(c, y) \equiv C_k^{(2)\Lambda}(r = \|x - y\|)$ for a translationally invariant fluid. Note that the right hand side is non singular since the denominator is negative definite. It is a general property that the flow of f_k^Λ has neither UV or IR singularities, in particular IR singularities (near a critical point) are smoothened by k and they build up progressively as the scale-k is lowered[11, 12].

To make contact with the work of Reatto ‘et al.’ let me consider now the case of a sharp cut-off, *i. e.* $C(q, k) = 1 - \Theta(q - k)$. Then equation (40) becomes [13].

$$\partial_k f_k^\Lambda = \frac{k^{d-1}}{2} \frac{S_d}{(2\pi)^d} \ln \left\{ 1 - \frac{\tilde{w}_0^\Lambda(k)}{\tilde{\mathcal{C}}_k^{(2)\Lambda}(k)} \right\}, \quad (41)$$

where $S_d = 2\pi^{d/2}/\Gamma(d/2)$. This is the usual HRT equation [6]. In order to obtain (41) from (40) one replaces the sharp $\Theta(q - k)$ by a smooth one,

$\Theta_\epsilon(q, k)$, denotes $\delta_\epsilon(q, k) = -\partial_k \Theta_\epsilon(q, k)$ the smooth δ -function and finally make use of Morris lemma which states that, for $\epsilon \rightarrow 0$

$$\delta_\epsilon(q, k) f(\Theta_\epsilon(q, k), k) \rightarrow \delta(q - k) \int_0^1 dt f(t, q), \quad (42)$$

provided that the function $f(\Theta_\epsilon(q, k), k)$ is continuous at $k = q$ in the limit $\epsilon \rightarrow 0$, which is the case here. In the canonical field KSSHE theory for liquids one needs to consider rather an ultra-sharp cut-off regulator [13].

Whatever the considered version of HRT, smooth or sharp cut-off, *i. e.* respec. equations (40) and (41), both equations are of a formidable complexity despite their apparent simplicity. Indeed the kernels of these PDE involve the two-body $C_k^{(2)\Lambda}[\rho]$ which depends **functionally** on the density. Clearly one can deduce from these equations an infinite tower of equations for the $C_k^{(n)\Lambda}[\rho]$ ($1, \dots, n$) by differentiating them functionally with respect to the density profile $\rho(x)$. A discussion of this point is however out the scope of the present paper, it has been developed in detail in a general context in reference [13].

5 Conclusion

In this paper I have developed a new version of the “smooth” hierarchical reference theory for liquids. It can be seen as an effort to conciliate the point of view of the theory of liquids and that of statistical field theory. Technically it is an application to a peculiar field theory (KSSHE), aimed at representing liquids, of the more general theory developed in reference [13]. The equivalence pair potentials \leftrightarrow propagators is the crux of the whole matter. In addition, the interplay between the points of view of Wilson and Wetterich in their application to the theory of liquids yields a better understanding of the work of Reatto and his collaborators.

From a prosaic point of view the differences with the first version of this work [19] are small but with interesting consequences. In practice, if one leaves aside philosophical considerations on Wilsonian and Wetterich actions, the main changes concern essentially the expression of the pair potential w_k^Λ of the k -system. In the first version, following Wetterich, I add a mass term $\varphi \cdot \mathcal{R}_k \cdot \varphi/2$ to the KSSHE action. With $\mathcal{R}_k(q) \sim Zk^2(1 - \Theta_\epsilon(q, k))$, Z large. This results in an ugly pair potential for the k -system, of the form $\tilde{w}_k^\Lambda(q) = \tilde{w}_0^\Lambda(q)/(1 + \tilde{w}_0^\Lambda(q)\mathcal{R}_k(q))$. In order to recover Reatto’s equation (41) one then needs to consider an ultra-sharp cut-off limit, *i. e.* : $\epsilon \rightarrow 0$ and $Z \rightarrow \infty$. I recall that, here, only the simple sharp cut-off limit $\epsilon \rightarrow 0$, ($Z = 1$) is required.

In the present formalism well-chosen cut-off functions such as $\overline{C}(x) = \exp(-x^2/2)$ yields analytical $w_k^\Lambda(r)$ in many cases, for instance $w(r) = \exp(-ar)/r$ (Yukawa), $w(r) = 1/r^{d+n}$, etc. Indeed one then obtains for $w_k^\Lambda(r) \equiv w_{\text{Ewald}}(r)$ nothing but the Ewald potential in direct space, the guy of numerical simulations. The lacking contribution in Fourier space corresponds to interactions between “blocks” of size $1/k$. This potential $w_{\text{Ewald}}(r)$ is monotonous in general. In the old version the potential $w_k^\Lambda(r)$ is not analytical and oscillates in direct space.

A last difference can be emphasized : in the old version the initial condition for the flow equation of $\beta\mathcal{A}_k^\Lambda$ requires that the cut-off function $\mathcal{R}_\Lambda = \infty$, which is difficult to implement rigorously in practice and could lead to unexpected errors in numerical applications. In the present version, as discussed in section 4.3 there is no such problem and the initial condition is easily implemented.

Despite the beauty and success of Reatto’s HRT some drawbacks of the theory appeal a smooth cut-off version of it, such as the one exposed here. A sharp cut-off regulator induces singularities in the pair potential $w_k^\Lambda(r)$ which decays slowly as $\sim \cos(kr)/r$ for $r \rightarrow \infty$. This circumstance makes it difficult to solve exactly the integral equations involved in the most widely used closures of the Hierarchy; one has to resort to approximations which, as discussed by Reiner [27] are sometimes not easy to controll. A second drawback of the sharp cut-off version is the value of some critical exponents, notably that of the specific heat, $\alpha \sim -0.05$, which is negative, while positive as it should in the smooth cut-off version [28].

It seems to me that solving exactly the smooth cut-off version of HRT is possible; that is coupling the numerical solution of a PDE (flow equation) and integral equations (closure of the hierarchy). Some of the drawbacks of the Reatto’s ‘et al’ version of HRT could then be cured.

Acknowledgments

This paper was written in honour of L. Reatto.

A Alternative derivation of the RG flow of W_k^Λ

I derive the flow of W_k^Λ in the framework of field theory (see also reference[13]). I will start from equation (22b)

$$\begin{aligned} L &= R \\ \Xi_k^\Lambda[\nu_k = \nu + w_k^\Lambda(0)/2] &= e^{D_k^\Lambda} \Xi_{(\text{HS})}[\nu] , \end{aligned} \quad (43)$$

and take the partial derivatives of the both sides “ L ” and “ R ” of EQ. (43) with respect to the scale “ k ”. One thus has for the l.h.s.

$$\begin{aligned} \partial_k L|_\nu &= \partial_k \Xi_k^\Lambda[\nu_k] + \int_\Omega d^d x \frac{\delta \Xi_k^\Lambda}{\delta \nu_k} \partial_k \nu_k , \\ &= \Xi_k^\Lambda[\nu_k] \times \left\{ \partial_k W_k^\Lambda[\nu_k] + \frac{1}{2} \int_\Omega d^d x W_k^{(1)\Lambda}[\nu_k](x) \partial_k w_k^\Lambda(0)/2 \right\} , \end{aligned} \quad (44)$$

and, for the r.h.s.

$$\begin{aligned} \partial_k R|_\nu &= \partial_k D_k^\Lambda e^{D_k^\Lambda} \Xi_{(\text{HS})}[\nu] \\ &= \frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_k^\Lambda(x, y) \frac{\delta^2 \Xi_k^\Lambda[\nu_k]}{\delta \nu_k(x) \delta \nu_k(y)} \\ &= \Xi_k^\Lambda[\nu_k] \times \frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_k^\Lambda(x, y) G_k^\Lambda[\nu_k](x, y) , \end{aligned} \quad (45)$$

where I used the expression :

$$D_k^\Lambda \dots = \frac{1}{2} \int_\Omega d^d x d^d y w_k^\Lambda(x, y) \frac{\delta^2 \dots}{\delta \nu_k(x) \delta \nu_k(y)} . \quad (46)$$

Equating equations (44) and (45) and noting that the equality, obtained for arbitrary ν_k , is then valid in the change $\nu_k \rightarrow \nu$, ν arbitrary, one obtains finally

$$\partial_k W_k^\Lambda[\nu]|_\nu = \frac{1}{2} \int_\Omega d^d x d^d y \partial_k w_k^\Lambda(x, y) \left\{ G_k^\Lambda(x, y) - \rho_k^\Lambda(x) \delta^{(d)}(x - y) \right\} , \quad (47)$$

which indeed coincides with equation(25).

B Mean field theory at scale “ k ”

The Mean-Field approximation of the GCPF of the k -system will be defined as

$$\Xi_k^{\Lambda(\text{MF})}[\nu] \triangleq \exp \left\{ -\frac{1}{2} \varphi^\star \cdot R_k^\Lambda \cdot \varphi^\star + W_{(\text{HS})}[\nu_k + \varphi^\star] \right\} , \quad (48)$$

where $\nu_k = \nu - w_k^\Lambda(0)/2$ and φ^\star is the location of the saddle point integrand (17b). φ^\star satisfies the implicit relation

$$\begin{aligned} R_k^\Lambda \cdot \varphi^\star &= \frac{\delta}{\delta \varphi^\star} W_{(\text{HS})}[\nu_k + \varphi^\star] \\ &= \rho_{(\text{HS})}[\nu_k + \varphi^\star](x) . \end{aligned} \quad (49)$$

For a given chemical potential $\nu(x)$ the MF profile of the k-system is given by $\rho_k^{\Lambda(\text{MF})}(x) = \delta \ln \Xi_k^{\Lambda(\text{MF})}[\nu] / \delta \nu(x) = \rho_{(\text{HS})}[\nu_k + \varphi^\star](x)$ where I made use of the stationary condition (49). Therefore the “true” Kohn-Sham free energy of the k-system is given by

$$\beta \overline{\mathcal{A}}_k^{\Lambda(\text{MF})} = -\ln \Xi_k^{\Lambda(\text{MF})} + \nu \cdot \rho_k^{\Lambda(\text{MF})} . \quad (50)$$

A short calculation will show that [19, 13]

$$\beta \overline{\mathcal{A}}_k^{\Lambda(\text{MF})}[\rho] = \beta \mathcal{A}_{(\text{HS})}[\rho] - \frac{1}{2} \rho \cdot w_k^\Lambda \cdot \rho + \frac{1}{2} \rho \cdot w_k^\Lambda(0) . \quad (51)$$

where $\beta \mathcal{A}_{(\text{HS})}[\rho]$ is the free energy functional of the HS fluid at same density. Therefore one finds for the average effective Kohn-Sham free energy

$$\beta \mathcal{A}_k^{\Lambda(\text{MF})}[\rho] = \beta \mathcal{A}_{(\text{HS})}[\rho] - \frac{1}{2} \rho \cdot w_0^\Lambda \cdot \rho + \frac{1}{2} \rho \cdot w_0^\Lambda(0) . \quad (52)$$

Note that $\beta \mathcal{A}_k^{\Lambda(\text{MF})}[\rho]$ is independent of scale “k” and thus equal to its initial value $\beta \mathcal{A}_\Lambda^{\Lambda(\text{MF})}[\rho]$.

I prove now that $\beta \overline{\mathcal{A}}_k^{\Lambda(\text{MF})}[\rho]$ is a rigorous upper bound to the Kohn-Sham free energy of the k-system [26, 18]. We consider the Legendre-Fenchel relation for the reference system of hard spheres :

$$W_{(\text{HS})}[\nu] = \sup_{\rho} \{ \nu \cdot \rho - \beta \mathcal{A}_{(\text{HS})}[\rho] \} \quad (\forall \nu) \quad (53)$$

which implies the Young inequalities

$$(\forall \nu, \forall \rho) \quad W_{(\text{HS})}[\nu] + \beta \mathcal{A}_{(\text{HS})}[\rho] \geq \rho \cdot \nu . \quad (54)$$

Injecting this inequality in the expression (17b) of $\Xi_k^\Lambda[\nu]$ one gets $(\forall \nu, \forall \rho)$

$$\begin{aligned} \Xi_k^\Lambda[\nu] &\geq \exp(-\beta \mathcal{A}_{(\text{HS})}[\rho] + \rho \cdot \nu_k) \int \frac{\mathcal{D}\varphi}{\mathcal{N}_{w_k^\Lambda}} \exp(-\frac{1}{2} \varphi \cdot R_k^\Lambda \cdot \varphi + \rho \cdot \varphi) \\ &\geq \exp(-\beta \mathcal{A}_{(\text{HS})}[\rho] + \rho \cdot \nu_k + \frac{1}{2} \rho \cdot w_k^\Lambda \cdot \rho) , \end{aligned} \quad (55)$$

where I made use of Wick’s theorem. Rearranging the terms one thus has

$$(\forall \nu, \forall \rho) \quad \rho \cdot \nu - W_k^\Lambda[\nu] \leq \beta \overline{\mathcal{A}}_k^{\Lambda(\text{MF})}[\rho] , \quad (56)$$

and thus

$$(\forall \rho) \quad \beta \overline{\mathcal{A}}_k^{\Lambda(\text{MF})}[\rho] \geq \sup_{\nu} \{ \rho \cdot \nu - W_k^\Lambda[\nu] \} . \quad (57)$$

Hence, from the very definition of the Legendre transform (28b)

$$(\forall \rho) \quad \beta \overline{\mathcal{A}}_k^{\Lambda(\text{MF})}[\rho] \geq \beta \overline{\mathcal{A}}_k^\Lambda[\rho] \quad (58)$$

Turning now our attention to the effective average Kohn-Sham free energy I find the exact upper bound :

$$(\forall \rho) \quad \beta \mathcal{A}_k^{\Lambda(\text{MF})}[\rho] = \beta \mathcal{A}_\Lambda^\Lambda[\rho] \geq \beta \mathcal{A}_k^\Lambda[\rho]. \quad (59)$$

References

- [1] K. G. Wilson and J. Kogut, *Phys. Rep. C* **12**, 77 (1974).
- [2] F. J. Wegner, *Phase Transitions and Critical Phenomena Vol. VI*, Domb C and Green M S eds (Academic Press, New York, 1976).
- [3] A. Parola and L. Reatto, *Phys. Rev. Lett.* **53**, 2417 (1984).
- [4] A. Parola and L. Reatto, *J. Stat. Phys.* **72**, 1179 (1985).
- [5] A. Parola, *J. Phys. C:Solid State Phys.* **19**, 5071 (1986).
- [6] A. Parola and L. Reatto, *Adv. Phys.* **44**, 211 (1995).
- [7] A. Parola, D. Pini and L. Reatto, *Mol. Phys.* **107**, 503 (2009).
- [8] J. Polchinski, *Nucl. Phys. B* **231**, 269 (1984).
- [9] C. Bervillier and C. Bagnuls, *Phys. Rep.* **348**, 91 (2001)
- [10] Tim R Morris, *Int. J. Mod. Phys. A* **9**, 2411 (1994).
- [11] Berges J. Berges, N.Tetradis, and C. Wetterich, *Phys. Rep.* **363** (2002).
- [12] B. Delamotte, *Order, Disorder and Criticality. Advanced Problems of Phase Transition Theory*, Vol. **II**, Y. Holovatch ed. (World Scientific, Singapore, 2007).
- [13] J.-M. Caillol, *J. Phys. A : Math. Gen.* **42**, 225004 (2009).
- [14] R. L. Stratonovich, *Sov. Phys. Solid State* **2**, 1824 (1958).
- [15] J. Hubbard, *Phys. Rev. Lett.* **3**, 77 (1954).
- [16] N. V. Brilliantov, *Phys. Rev. E* **58**, 2628 (1998).
- [17] Hyung-June and Song Xueyu, *J. Chem. Phys.* **114**, 5637 (2001).
- [18] J.-M. Caillol, *Mol. Phys.* **101**, 1617 (2003).
- [19] J.-M. Caillol, *Mol. Phys.* **104**, 1931 (2006).
- [20] M. Kac, *Phys. Fluids*, **2**, 8 (1959)
- [21] A. J. F. Siegert, *Physica*, **26**, 530 (1960).
- [22] S. F. Edwards, *Phil. Mag.*, **4**, 1171 (1959).
- [23] J.-P. Hansen and I. R. Mc Donald 1986, *Theory of Simple Liquids*. (London : Academic Press).
- [24] D. Ruelle 1969, *Statistical mechanics, rigorous results*. (Benjamin).
- [25] N. Goldenfeld 1992, *Lectures on Phase Transitions and the Renormalization Group* (Addison-Wesley).
- [26] J.-M. Caillol, *J. Phys. A : Math. Gen.* **35**, 4189 (2002).
- [27] A. Reiner and G. Kahl, *Phys. Rev. E* **65**, 046701 (2002).
- [28] J. M. Caillol, *submitted*.